

Claims

What is claimed is:

1. A method of determining ElogD_{oct} for chemical compounds which comprises:
 - a. Introducing said chemical compounds seriatim to the column of a reverse phase high performance liquid chromatographic system said column being an embedded amide functional group column; or a C-18 bonded column with low silanol activity; and
 - b. Eluting said compounds with a mobile phase containing MOPS buffer and a methanol/octanol mixture in which the proportions of said methanol/octanol mixture to said buffer are from 75 to 15% v/v; and with flow rates between 0.5 and 3 ml/min and
 - c. Measuring the retention time required to elute each sample from said column; and
 - d. Calculating ElogD_{oct} from the retention time of each sample using equation 1:
$$\log D_{oct} = 1.1267 (\pm 0.0233) \log k_w + 0.2075 (\pm 0.0430) \quad (\text{Eq. 1}).$$
- 15 2. The method of claim 1 wherein said compounds for which ElogD_{oct} is to be determined are divided into groups according to calculated lipophilicity based on chemical structure and; ElogD_{oct} is determined for all samples in a first group and; said column is equilibrated to the conditions for a second group.
- 20 3. The method of claim 1 wherein each of steps a) through d) is performed by robotic means under the control of a programmed computer.
4. The method of claim 1 wherein said column is an embedded amide functional group column.
5. The method of claim 1 wherein said column is a C-18 bonded column with low silanol activity.
- 25 6. The method of claim 1 wherein the buffer pH is between 4 and 8.